Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2024 – 04:56 AM EST

PDB ID	:	4IST
Title	:	S177A Kluyveromyces lactis Allophanate Hydrolase
Authors	:	Fan, C.; Xiang, S.
Deposited on	:	2013-01-17
Resolution	:	2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

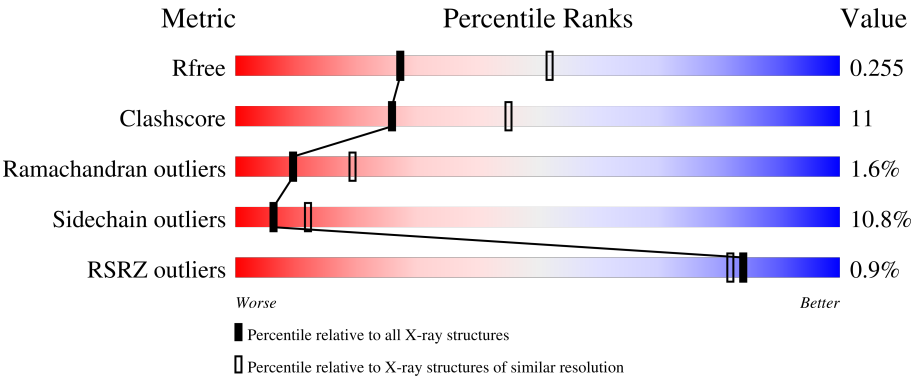
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

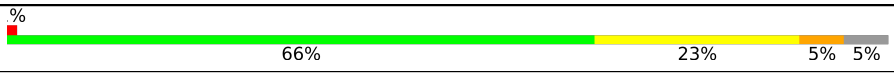
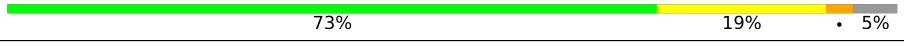
The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	644	
1	B	644	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9652 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Allophanate Hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	614	Total	C	N	O	S	0	0	0
			4747	3051	786	896	14			
1	B	614	Total	C	N	O	S	0	0	0
			4747	3051	786	896	14			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	expression tag	UNP Q6CP22
A	-21	GLY	-	expression tag	UNP Q6CP22
A	-20	SER	-	expression tag	UNP Q6CP22
A	-19	SER	-	expression tag	UNP Q6CP22
A	-18	HIS	-	expression tag	UNP Q6CP22
A	-17	HIS	-	expression tag	UNP Q6CP22
A	-16	HIS	-	expression tag	UNP Q6CP22
A	-15	HIS	-	expression tag	UNP Q6CP22
A	-14	HIS	-	expression tag	UNP Q6CP22
A	-13	HIS	-	expression tag	UNP Q6CP22
A	-12	SER	-	expression tag	UNP Q6CP22
A	-11	SER	-	expression tag	UNP Q6CP22
A	-10	GLY	-	expression tag	UNP Q6CP22
A	-9	LEU	-	expression tag	UNP Q6CP22
A	-8	VAL	-	expression tag	UNP Q6CP22
A	-7	PRO	-	expression tag	UNP Q6CP22
A	-6	ARG	-	expression tag	UNP Q6CP22
A	-5	GLY	-	expression tag	UNP Q6CP22
A	-4	SER	-	expression tag	UNP Q6CP22
A	-3	HIS	-	expression tag	UNP Q6CP22
A	-2	MET	-	expression tag	UNP Q6CP22
A	-1	ALA	-	expression tag	UNP Q6CP22
A	0	SER	-	expression tag	UNP Q6CP22
A	177	ALA	SER	engineered mutation	UNP Q6CP22
B	-22	MET	-	expression tag	UNP Q6CP22

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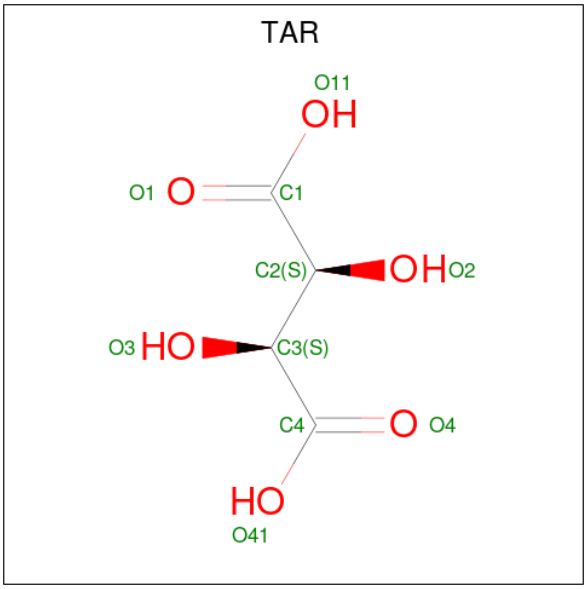
Chain	Residue	Modelled	Actual	Comment	Reference
B	-21	GLY	-	expression tag	UNP Q6CP22
B	-20	SER	-	expression tag	UNP Q6CP22
B	-19	SER	-	expression tag	UNP Q6CP22
B	-18	HIS	-	expression tag	UNP Q6CP22
B	-17	HIS	-	expression tag	UNP Q6CP22
B	-16	HIS	-	expression tag	UNP Q6CP22
B	-15	HIS	-	expression tag	UNP Q6CP22
B	-14	HIS	-	expression tag	UNP Q6CP22
B	-13	HIS	-	expression tag	UNP Q6CP22
B	-12	SER	-	expression tag	UNP Q6CP22
B	-11	SER	-	expression tag	UNP Q6CP22
B	-10	GLY	-	expression tag	UNP Q6CP22
B	-9	LEU	-	expression tag	UNP Q6CP22
B	-8	VAL	-	expression tag	UNP Q6CP22
B	-7	PRO	-	expression tag	UNP Q6CP22
B	-6	ARG	-	expression tag	UNP Q6CP22
B	-5	GLY	-	expression tag	UNP Q6CP22
B	-4	SER	-	expression tag	UNP Q6CP22
B	-3	HIS	-	expression tag	UNP Q6CP22
B	-2	MET	-	expression tag	UNP Q6CP22
B	-1	ALA	-	expression tag	UNP Q6CP22
B	0	SER	-	expression tag	UNP Q6CP22
B	177	ALA	SER	engineered mutation	UNP Q6CP22

- Molecule 2 is D(-)-TARTARIC ACID (three-letter code: TAR) (formula: $C_4H_6O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 10 4 6	0	0
2	B	1	Total C O 10 4 6	0	0

- Molecule 3 is water.

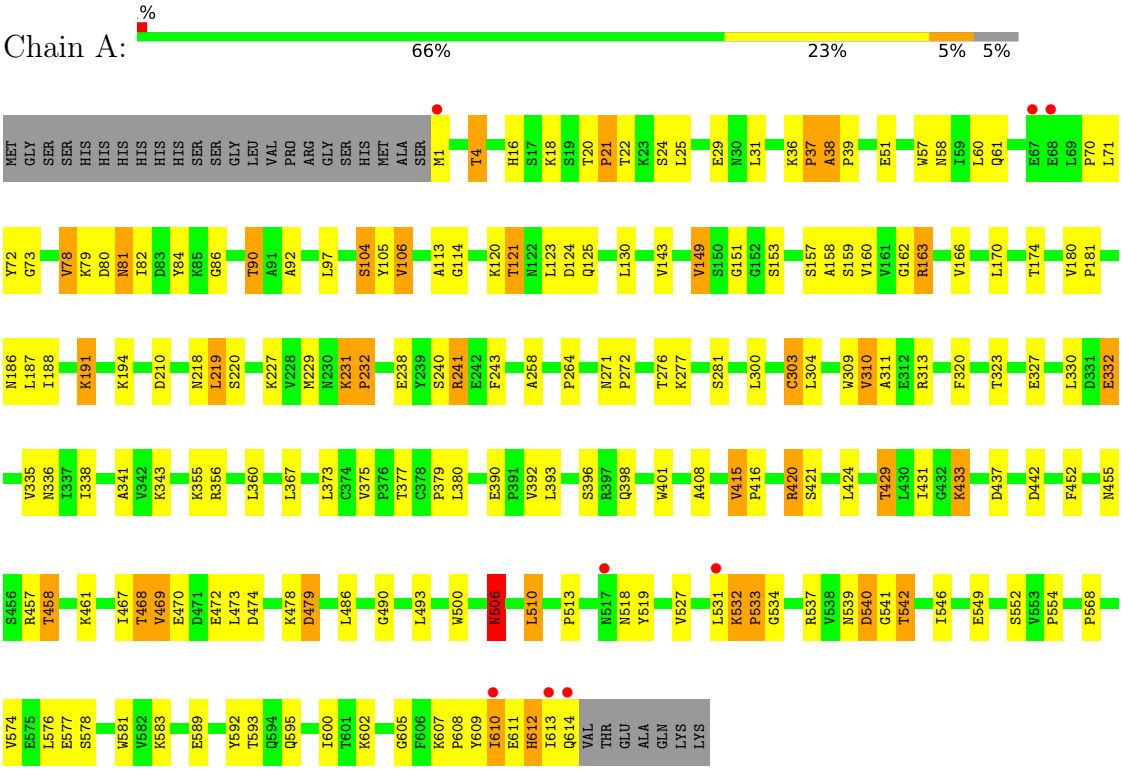
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	59	Total O 59 59	0	0
3	B	79	Total O 79 79	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

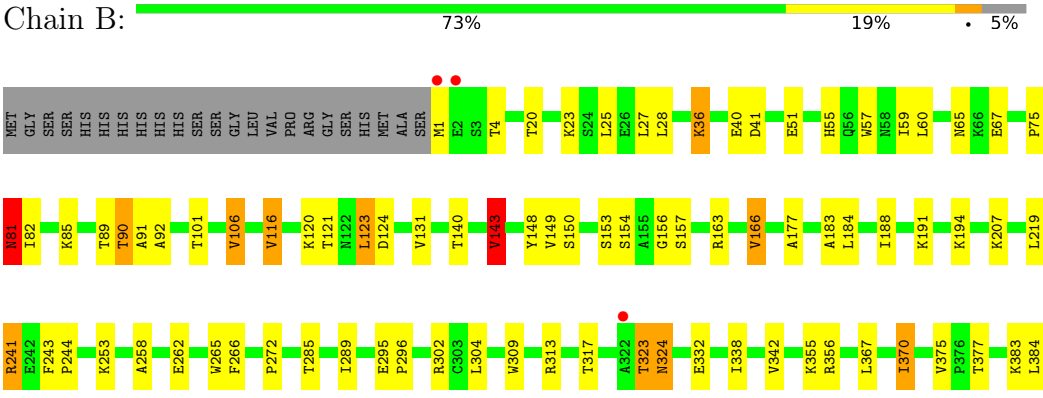
• Molecule 1: Allophanate Hydrolase

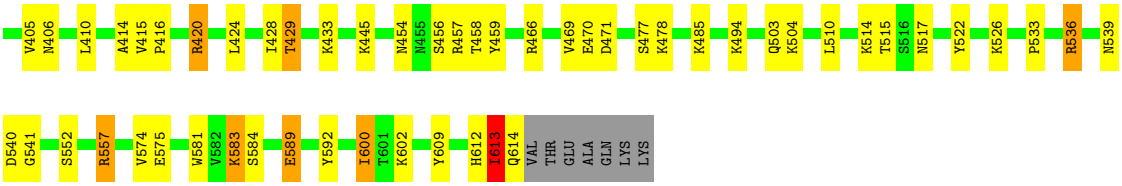
Chain A:



• Molecule 1: Allophanate Hydrolase

Chain B:




V405
N406
L410
A414
V415
P416
R420
L424
I428
T429
K433
K445
N454
N455
S456
R457
T458
Y459
R466
V469
E470
D471
S477
K478
K485
K494
Q503
K504
L510
K514
T515
S516
N517
Y522
K526
P533
R536
N539

D540
G541
S552
R557
V574
E575
W581
V582
K583
S584
E589
Y592
I600
T601
K602
Y609
H612
I613
Q614
VAL
THR
GLU
ALA
GLN
LYS
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	89.90Å 107.40Å 152.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.01 – 2.60 40.01 – 2.60	Depositor EDS
% Data completeness (in resolution range)	93.0 (40.01-2.60) 93.1 (40.01-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.44 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.184 , 0.256 0.184 , 0.255	Depositor DCC
R_{free} test set	2187 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	45.1	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 29.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9652	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TAR

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.71	3/4861 (0.1%)	0.86	1/6617 (0.0%)
1	B	0.71	2/4861 (0.0%)	0.86	6/6617 (0.1%)
All	All	0.71	5/9722 (0.1%)	0.86	7/13234 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	309	TRP	CD2-CE2	6.62	1.49	1.41
1	A	500	TRP	CD2-CE2	6.45	1.49	1.41
1	A	581	TRP	CD2-CE2	5.42	1.47	1.41
1	B	57	TRP	CD2-CE2	5.34	1.47	1.41
1	B	309	TRP	CD2-CE2	5.27	1.47	1.41

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	241	ARG	NE-CZ-NH1	8.05	124.32	120.30
1	B	367	LEU	CA-CB-CG	7.95	133.58	115.30
1	B	557	ARG	NE-CZ-NH2	-6.81	116.89	120.30
1	B	557	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	B	81	ASN	N-CA-CB	-5.79	100.18	110.60
1	B	241	ARG	NE-CZ-NH2	-5.56	117.52	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	163	ARG	NE-CZ-NH1	5.44	123.02	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	37	PRO	Peptide
1	A	468	THR	Peptide
1	A	539	ASN	Peptide
1	A	612	HIS	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4747	0	4774	118	0
1	B	4747	0	4774	87	0
2	A	10	0	4	0	0
2	B	10	0	4	0	0
3	A	59	0	0	6	0
3	B	79	0	0	4	0
All	All	9652	0	9556	201	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (201) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:ALA:HB1	1:A:39:PRO:HD2	1.19	1.14
1:A:38:ALA:HB1	1:A:39:PRO:CD	1.81	1.11
1:B:90:THR:HG22	1:B:92:ALA:H	1.20	1.07
1:A:38:ALA:CB	1:A:39:PRO:HD2	1.85	1.05
1:A:220:SER:HB2	1:A:470:GLU:O	1.65	0.96
1:A:532:LYS:H	1:A:532:LYS:HE2	1.30	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:LYS:HG2	1:A:81:ASN:HB2	1.53	0.89
1:A:79:LYS:HA	1:A:121:THR:HG22	1.56	0.87
1:A:612:HIS:HB2	3:A:826:HOH:O	1.74	0.86
1:A:121:THR:HG21	1:A:157:SER:OG	1.75	0.85
1:A:336:ASN:HB3	3:A:848:HOH:O	1.77	0.84
1:A:592:TYR:OH	1:B:589:GLU:HG3	1.79	0.82
1:B:377:THR:OG1	1:B:429:THR:HG22	1.80	0.81
1:A:332:GLU:HB3	3:A:818:HOH:O	1.80	0.80
1:A:320:PHE:O	1:A:323:THR:HB	1.82	0.79
1:A:16:HIS:ND1	1:A:24:SER:HB2	1.97	0.79
1:B:143:VAL:CG2	1:B:163:ARG:HG3	2.12	0.79
1:A:241:ARG:HG3	3:A:810:HOH:O	1.83	0.77
1:B:90:THR:CG2	1:B:92:ALA:H	1.97	0.76
1:A:607:LYS:HB2	1:A:608:PRO:HD3	1.68	0.74
1:B:90:THR:HG22	1:B:92:ALA:N	2.01	0.71
1:A:232:PRO:O	1:A:240:SER:OG	2.06	0.71
1:B:121:THR:HG21	1:B:157:SER:OG	1.92	0.70
1:A:16:HIS:CE1	1:A:24:SER:HB2	2.28	0.69
1:B:106:VAL:HG22	1:B:229:MET:HG2	1.73	0.69
1:A:162:GLY:HA2	1:A:187:LEU:HD21	1.73	0.68
1:A:420:ARG:HG3	1:A:424:LEU:O	1.94	0.67
1:B:131:VAL:O	1:B:149:VAL:HG13	1.95	0.66
1:B:600:ILE:HD11	1:B:609:TYR:CE1	2.31	0.65
1:A:36:LYS:HE2	3:A:859:HOH:O	1.98	0.64
1:A:373:LEU:HB2	1:A:431:ILE:HB	1.79	0.64
1:A:57:TRP:O	1:A:61:GLN:HG2	1.97	0.63
1:A:58:ASN:O	1:A:61:GLN:HB2	1.98	0.63
1:B:522:TYR:O	1:B:533:PRO:HA	1.99	0.63
1:A:600:ILE:HD11	1:A:609:TYR:CD1	2.34	0.63
1:A:493:LEU:HD23	1:A:549:GLU:HB2	1.80	0.62
1:B:536:ARG:HG3	1:B:592:TYR:CZ	2.35	0.62
1:A:191:LYS:O	1:A:191:LYS:HE3	2.01	0.61
1:A:84:TYR:CE2	1:A:86:GLY:HA3	2.36	0.60
1:A:38:ALA:CB	1:A:39:PRO:CD	2.49	0.60
1:A:79:LYS:C	1:A:81:ASN:H	2.04	0.59
1:A:124:ASP:HB2	1:A:153:SER:HB3	1.84	0.58
1:A:367:LEU:O	1:A:433:LYS:NZ	2.36	0.58
1:B:504:LYS:O	1:B:504:LYS:HG2	2.02	0.58
1:A:78:VAL:HG22	1:A:120:LYS:HE2	1.85	0.58
1:B:456:SER:HA	1:B:466:ARG:HD2	1.86	0.56
1:B:90:THR:CG2	1:B:92:ALA:N	2.63	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:ASP:OD1	1:A:90:THR:HG22	2.06	0.56
1:A:60:LEU:HD22	1:A:72:TYR:CE1	2.41	0.56
1:A:416:PRO:HG2	1:A:457:ARG:HH21	1.69	0.56
1:A:610:ILE:O	1:A:614:GLN:HG3	2.06	0.56
1:B:258:ALA:HB2	1:B:370:ILE:HG12	1.88	0.56
1:B:504:LYS:NZ	3:B:855:HOH:O	2.39	0.56
1:B:420:ARG:HD3	1:B:424:LEU:HB2	1.88	0.55
1:B:613:ILE:HG23	1:B:613:ILE:O	2.05	0.55
1:A:540:ASP:O	1:A:542:THR:N	2.37	0.55
1:A:227:LYS:HZ1	1:A:474:ASP:HB3	1.71	0.55
1:B:377:THR:HA	1:B:429:THR:CG2	2.37	0.55
1:A:78:VAL:HG23	1:A:82:ILE:HB	1.87	0.55
1:A:589:GLU:OE2	1:B:536:ARG:HD3	2.07	0.55
1:A:4:THR:HG21	1:A:31:LEU:HD13	1.88	0.55
1:B:79:LYS:HE3	1:B:154:SER:HA	1.88	0.55
1:A:532:LYS:HE2	1:A:532:LYS:N	2.12	0.54
1:A:90:THR:HG23	1:A:92:ALA:N	2.23	0.54
1:B:121:THR:OG1	1:B:156:GLY:HA3	2.07	0.54
1:A:188:ILE:HD13	1:A:218:ASN:C	2.28	0.54
1:B:405:VAL:HG13	1:B:410:LEU:HB2	1.90	0.53
1:B:143:VAL:HG22	1:B:163:ARG:HG3	1.89	0.52
1:A:106:VAL:CG1	1:A:229:MET:HE3	2.39	0.52
1:B:539:ASN:O	1:B:541:GLY:N	2.36	0.52
1:B:220:SER:HB3	1:B:470:GLU:O	2.10	0.52
1:B:140:THR:O	1:B:150:SER:HB3	2.10	0.52
1:A:90:THR:HG23	1:A:92:ALA:H	1.74	0.52
1:A:174:THR:OG1	1:A:210:ASP:OD1	2.29	0.51
1:B:79:LYS:HA	1:B:121:THR:HG22	1.91	0.51
1:A:271:ASN:N	1:A:272:PRO:HD2	2.25	0.51
1:B:124:ASP:HB2	1:B:153:SER:HB2	1.93	0.50
1:B:265:TRP:CD2	1:B:272:PRO:HG3	2.46	0.50
1:B:503:GLN:HB3	3:B:825:HOH:O	2.12	0.50
1:B:510:LEU:HD11	1:B:552:SER:HB2	1.94	0.49
1:B:253:LYS:HE2	1:B:285:THR:O	2.12	0.49
1:B:91:ALA:HA	1:B:123:LEU:HD11	1.94	0.49
1:A:78:VAL:HG22	1:A:120:LYS:CE	2.42	0.49
1:A:589:GLU:HG3	1:B:589:GLU:CG	2.42	0.49
1:A:188:ILE:CD1	1:A:218:ASN:HA	2.43	0.49
1:B:183:ALA:HB2	1:B:377:THR:HG21	1.94	0.49
1:A:130:LEU:HD22	1:A:180:VAL:HG21	1.95	0.48
1:A:180:VAL:HB	1:A:181:PRO:HD3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:LEU:HD21	1:A:408:ALA:HA	1.95	0.48
1:B:323:THR:O	1:B:324:ASN:C	2.52	0.48
1:A:79:LYS:CA	1:A:121:THR:HG22	2.38	0.48
1:A:452:PHE:CD1	1:A:457:ARG:HG3	2.49	0.48
1:B:75:PRO:HB2	1:B:166:VAL:HG23	1.94	0.48
1:B:612:HIS:C	1:B:614:GLN:H	2.17	0.48
1:A:106:VAL:CG1	1:A:229:MET:CE	2.91	0.48
1:B:143:VAL:HG23	1:B:163:ARG:HG3	1.95	0.47
1:A:540:ASP:C	1:A:542:THR:H	2.18	0.47
1:A:106:VAL:HG13	1:A:229:MET:CE	2.45	0.47
1:B:153:SER:H	1:B:177:ALA:CB	2.27	0.47
1:B:613:ILE:O	1:B:613:ILE:CG2	2.62	0.47
1:A:330:LEU:HB3	1:A:335:VAL:HG21	1.97	0.47
1:A:90:THR:CG2	1:A:92:ALA:H	2.27	0.47
1:A:106:VAL:HG11	1:A:229:MET:HE3	1.97	0.46
1:A:611:GLU:HA	1:A:614:GLN:HB2	1.97	0.46
1:B:67:GLU:HB3	3:B:846:HOH:O	2.16	0.46
1:A:80:ASP:OD1	1:A:90:THR:CG2	2.64	0.46
1:B:78:VAL:O	1:B:120:LYS:HA	2.15	0.46
1:A:610:ILE:O	1:A:610:ILE:HG12	2.16	0.46
1:B:148:TYR:CE2	1:B:383:LYS:HG3	2.50	0.46
1:B:377:THR:CB	1:B:429:THR:HG22	2.45	0.46
1:A:25:LEU:O	1:A:29:GLU:HB2	2.16	0.46
1:B:79:LYS:C	1:B:81:ASN:H	2.19	0.46
1:B:445:LYS:HE2	1:B:445:LYS:HB3	1.74	0.46
1:B:191:LYS:HE3	1:B:406:ASN:OD1	2.16	0.46
1:A:38:ALA:HB3	1:A:39:PRO:HD2	1.89	0.46
1:A:546:ILE:HG23	1:A:605:GLY:HA2	1.98	0.46
1:B:458:THR:HG22	1:B:459:TYR:N	2.31	0.45
1:B:75:PRO:HA	1:B:116:VAL:O	2.16	0.45
1:B:36:LYS:O	1:B:41:ASP:HB3	2.17	0.45
1:B:515:THR:HG22	1:B:574:VAL:HG21	1.99	0.45
1:A:73:GLY:N	1:A:114:GLY:O	2.47	0.45
1:A:191:LYS:HE3	1:A:191:LYS:C	2.38	0.45
1:A:513:PRO:HG2	1:A:576:LEU:HD22	1.99	0.45
1:B:143:VAL:HG22	1:B:163:ARG:CG	2.47	0.45
1:B:370:ILE:O	1:B:433:LYS:NZ	2.43	0.44
1:B:55:HIS:O	1:B:59:ILE:HG13	2.18	0.44
1:B:153:SER:H	1:B:177:ALA:HB1	1.82	0.44
1:B:377:THR:HA	1:B:429:THR:HG23	1.99	0.44
1:B:414:ALA:HA	1:B:429:THR:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:519:TYR:CE2	1:A:537:ARG:HB2	2.53	0.44
1:A:589:GLU:HA	1:A:592:TYR:CZ	2.53	0.44
1:B:123:LEU:HD23	1:B:123:LEU:N	2.32	0.44
1:A:60:LEU:HA	1:A:60:LEU:HD23	1.80	0.43
1:B:295:GLU:HB3	1:B:296:PRO:HD3	2.00	0.43
1:B:78:VAL:HG23	1:B:82:ILE:HB	2.00	0.43
1:B:317:THR:HG21	1:B:338:ILE:HG21	1.99	0.43
1:A:124:ASP:HB2	1:A:153:SER:CB	2.47	0.43
1:A:231:LYS:HA	1:A:232:PRO:HD3	1.90	0.43
1:B:75:PRO:O	1:B:166:VAL:HG22	2.18	0.43
1:B:485:LYS:O	1:B:583:LYS:HB2	2.18	0.43
1:A:143:VAL:CG1	1:A:461:LYS:HB3	2.48	0.43
1:A:186:ASN:OD1	1:A:458:THR:HG22	2.18	0.43
1:A:540:ASP:OD1	1:A:542:THR:OG1	2.32	0.43
1:A:310:VAL:HG21	3:A:846:HOH:O	2.18	0.43
1:B:188:ILE:HD13	1:B:416:PRO:HD3	2.00	0.43
1:B:342:VAL:O	1:B:342:VAL:CG1	2.66	0.43
1:A:143:VAL:HG13	1:A:461:LYS:HB3	2.00	0.43
1:A:377:THR:HA	1:A:429:THR:HG23	2.00	0.43
1:A:607:LYS:HB2	1:A:608:PRO:CD	2.44	0.43
1:A:576:LEU:C	1:A:578:SER:N	2.72	0.42
1:B:20:THR:OG1	1:B:23:LYS:HG2	2.19	0.42
1:B:28:LEU:HD23	1:B:28:LEU:HA	1.95	0.42
1:A:162:GLY:CA	1:A:187:LEU:HD21	2.44	0.42
1:A:311:ALA:HA	1:A:341:ALA:HB2	2.02	0.42
1:A:379:PRO:HB2	1:A:380:LEU:HG	2.01	0.42
1:B:80:ASP:OD2	1:B:89:THR:HA	2.20	0.42
1:A:124:ASP:O	1:A:125:GLN:C	2.57	0.42
1:A:313:ARG:HB3	1:A:338:ILE:HG12	2.02	0.42
1:A:219:LEU:HB3	1:A:473:LEU:HD21	2.00	0.42
1:A:300:LEU:O	1:A:303:CYS:HB2	2.20	0.42
1:B:458:THR:CG2	1:B:459:TYR:N	2.83	0.42
1:B:539:ASN:CB	3:B:818:HOH:O	2.68	0.42
1:B:574:VAL:HG12	1:B:584:SER:HB2	2.02	0.42
1:B:65:ASN:N	1:B:65:ASN:OD1	2.53	0.41
1:B:124:ASP:HB2	1:B:153:SER:CB	2.50	0.41
1:A:258:ALA:HB3	1:A:373:LEU:HD23	2.01	0.41
1:A:390:GLU:O	1:A:392:VAL:N	2.53	0.41
1:A:149:VAL:HG13	1:A:151:GLY:H	1.86	0.41
1:A:415:VAL:HA	1:A:416:PRO:HD3	1.92	0.41
1:B:79:LYS:HA	1:B:121:THR:CG2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:THR:HB	1:A:21:PRO:HD2	2.03	0.41
1:A:398:GLN:OE1	1:A:398:GLN:HA	2.21	0.41
1:A:506:ASN:OD1	1:A:554:PRO:HG2	2.20	0.41
1:B:78:VAL:HG22	1:B:120:LYS:HE3	2.03	0.41
1:B:536:ARG:CG	1:B:592:TYR:CZ	3.03	0.41
1:B:149:VAL:HG23	1:B:384:LEU:HA	2.02	0.41
1:A:71:LEU:O	1:A:114:GLY:O	2.38	0.41
1:B:266:PHE:HZ	1:B:400:THR:HG21	1.86	0.41
1:B:504:LYS:O	1:B:557:ARG:NH2	2.53	0.41
1:A:106:VAL:HG13	1:A:229:MET:HE3	2.02	0.41
1:A:264:PRO:HD2	1:A:401:TRP:CZ2	2.56	0.41
1:A:455:ASN:HB3	1:A:467:ILE:O	2.21	0.41
1:B:81:ASN:HB3	1:B:82:ILE:HG13	2.02	0.41
1:B:457:ARG:HH21	1:B:471:ASP:CG	2.23	0.41
1:A:123:LEU:HA	1:A:153:SER:O	2.22	0.41
1:A:188:ILE:CD1	1:A:218:ASN:CA	2.99	0.40
1:A:533:PRO:HB2	1:A:534:GLY:H	1.66	0.40
1:A:158:ALA:O	1:A:187:LEU:HD11	2.21	0.40
1:A:490:GLY:HA3	1:A:533:PRO:CG	2.51	0.40
1:A:589:GLU:HG3	1:B:589:GLU:HG2	2.03	0.40
1:A:613:ILE:HG22	1:A:613:ILE:O	2.22	0.40
1:A:70:PRO:HD2	1:A:113:ALA:HB1	2.03	0.40
1:A:519:TYR:CZ	1:A:574:VAL:HG23	2.56	0.40
1:A:97:LEU:HD23	1:A:97:LEU:C	2.41	0.40
1:A:104:SER:O	1:A:105:TYR:C	2.59	0.40
1:A:311:ALA:HA	1:A:341:ALA:CB	2.52	0.40
1:A:486:LEU:HA	1:A:583:LYS:O	2.22	0.40
1:A:490:GLY:CA	1:A:533:PRO:HG3	2.51	0.40
1:A:510:LEU:CD1	1:A:552:SER:HB2	2.51	0.40
1:B:313:ARG:O	1:B:317:THR:HG22	2.22	0.40
1:B:575:GLU:HB2	1:B:581:TRP:CZ2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	612/644 (95%)	545 (89%)	53 (9%)	14 (2%)	6 11
1	B	612/644 (95%)	561 (92%)	46 (8%)	5 (1%)	19 39
All	All	1224/1288 (95%)	1106 (90%)	99 (8%)	19 (2%)	9 19

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	ALA
1	B	323	THR
1	B	540	ASP
1	A	479	ASP
1	A	541	GLY
1	A	577	GLU
1	B	143	VAL
1	B	613	ILE
1	A	533	PRO
1	A	21	PRO
1	A	276	THR
1	A	506	ASN
1	A	518	ASN
1	B	207	LYS
1	A	37	PRO
1	A	232	PRO
1	A	542	THR
1	A	610	ILE
1	A	469	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	523/548 (95%)	463 (88%)	60 (12%)	5 10
1	B	523/548 (95%)	470 (90%)	53 (10%)	7 14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1046/1096 (95%)	933 (89%)	113 (11%)	6 12

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	4	THR
1	A	18	LYS
1	A	22	THR
1	A	51	GLU
1	A	78	VAL
1	A	81	ASN
1	A	90	THR
1	A	104	SER
1	A	106	VAL
1	A	121	THR
1	A	149	VAL
1	A	159	SER
1	A	160	VAL
1	A	163	ARG
1	A	166	VAL
1	A	170	LEU
1	A	191	LYS
1	A	194	LYS
1	A	219	LEU
1	A	231	LYS
1	A	238	GLU
1	A	241	ARG
1	A	243	PHE
1	A	277	LYS
1	A	281	SER
1	A	303	CYS
1	A	304	LEU
1	A	310	VAL
1	A	327	GLU
1	A	332	GLU
1	A	343	LYS
1	A	355	LYS
1	A	356	ARG
1	A	375	VAL
1	A	393	LEU
1	A	396	SER

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Mol	Chain	Res	Type
1	A	415	VAL
1	A	420	ARG
1	A	421	SER
1	A	429	THR
1	A	433	LYS
1	A	437	ASP
1	A	442	ASP
1	A	458	THR
1	A	468	THR
1	A	469	VAL
1	A	472	GLU
1	A	478	LYS
1	A	479	ASP
1	A	506	ASN
1	A	510	LEU
1	A	527	VAL
1	A	531	LEU
1	A	532	LYS
1	A	540	ASP
1	A	568	PRO
1	A	593	THR
1	A	595	GLN
1	A	602	LYS
1	B	1	MET
1	B	4	THR
1	B	25	LEU
1	B	27	LEU
1	B	36	LYS
1	B	40	GLU
1	B	51	GLU
1	B	60	LEU
1	B	78	VAL
1	B	81	ASN
1	B	85	LYS
1	B	90	THR
1	B	101	THR
1	B	106	VAL
1	B	116	VAL
1	B	123	LEU
1	B	143	VAL
1	B	166	VAL
1	B	184	LEU

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Mol	Chain	Res	Type
1	B	194	LYS
1	B	219	LEU
1	B	241	ARG
1	B	243	PHE
1	B	244	PRO
1	B	262	GLU
1	B	289	ILE
1	B	302	ARG
1	B	304	LEU
1	B	324	ASN
1	B	332	GLU
1	B	355	LYS
1	B	356	ARG
1	B	370	ILE
1	B	375	VAL
1	B	393	LEU
1	B	415	VAL
1	B	420	ARG
1	B	428	ILE
1	B	429	THR
1	B	454	ASN
1	B	469	VAL
1	B	477	SER
1	B	478	LYS
1	B	494	LYS
1	B	514	LYS
1	B	517	ASN
1	B	526	LYS
1	B	536	ARG
1	B	583	LYS
1	B	589	GLU
1	B	600	ILE
1	B	602	LYS
1	B	613	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	455	ASN
1	B	81	ASN
1	B	186	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	TAR	B	701	-	9,9,9	1.17	0	12,12,12	1.26	2 (16%)
2	TAR	A	701	-	9,9,9	1.23	0	12,12,12	1.10	1 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TAR	B	701	-	-	6/12/12/12	-
2	TAR	A	701	-	-	4/12/12/12	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	701	TAR	O11-C1-C2	2.50	120.02	113.27
2	A	701	TAR	O11-C1-O1	-2.12	119.27	124.09
2	B	701	TAR	O3-C3-C2	-2.00	106.26	110.23

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	TAR	O3-C3-C4-O4
2	A	701	TAR	O3-C3-C4-O41
2	B	701	TAR	O3-C3-C4-O4
2	B	701	TAR	O3-C3-C4-O41
2	A	701	TAR	O1-C1-C2-O2
2	A	701	TAR	O11-C1-C2-O2
2	B	701	TAR	O1-C1-C2-O2
2	B	701	TAR	O11-C1-C2-C3
2	B	701	TAR	O1-C1-C2-C3
2	B	701	TAR	O11-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	614/644 (95%)	-0.32	8 (1%) 77 73	24, 44, 83, 164	0
1	B	614/644 (95%)	-0.43	3 (0%) 91 89	26, 42, 67, 120	0
All	All	1228/1288 (95%)	-0.38	11 (0%) 84 82	24, 43, 76, 164	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	614	GLN	9.3
1	A	610	ILE	3.3
1	A	1	MET	3.3
1	A	613	ILE	3.2
1	A	67	GLU	3.0
1	B	322	ALA	2.8
1	A	517	ASN	2.5
1	B	2	GLU	2.4
1	A	531	LEU	2.4
1	A	68	GLU	2.3
1	B	1	MET	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	TAR	B	701	10/10	0.92	0.23	53,63,67,68	0
2	TAR	A	701	10/10	0.94	0.17	49,53,60,63	0

6.5 Other polymers

There are no such residues in this entry.